

# DEHM Fact sheet

## 1.1 Assimilation and forecast system: synthesis of the main characteristics

<b>Discretisation</b>	Horizontal resolution	0.1° x 0.1° regular lat-lon
	Number of vertical levels	29
	Top altitude	100hPa
	Depth of lower most layer	20m
	Number of lower layers	12 below 1km
<b>Initial &amp; boundary conditions &amp; meteorology</b>	Meteorological driver	D-1 12:00 UTC IFS, 3hrly
	Boundary values	CAMS-Global IFS
	Initial values	Previous forecast
<b>Emissions: natural &amp; biogenic</b>	In-domain soil and road dust emissions	none
	In-domain sea-salt emissions	Mårtensson et al. (2003), Monahan et al. (1986)
	Birch, Grass, Olive, Ragweed, Alder, Mugwort Pollen provided by FMI	yes
	Biogenic emissions	MEGAN v2.04 (Gunther et. al 2006)
	Soil NOx	GEIA ( (Yienger and Levy, 1995)
	Wildfires emissions	last available 24h cycle over D-2 and D-1 cycled for AN (D-1) and FC (D+0 and D+1, zero for the remaining days)
<b>Chemistry/ Physics</b>	Gas phase chemistry	Modified Strand and Hov (1994), 74 species and 158 reactions
	Heterogeneous chemistry	Oxidation of NO <sub>2</sub> by O <sub>3</sub> on aerosols
	Aerosol size distribution	2 size fractions: PM <sub>2.5</sub> and coarse fraction of PM <sub>10</sub>
	Inorganic aerosols	Frohn (2004)
	Secondary organic aerosols	VBS approach (NPAS scheme of Bergström et al, 2012)
	Aqueous phase chemistry	SO <sub>2</sub> oxidation by O <sub>3</sub> and H <sub>2</sub> O <sub>2</sub> (Jonson et., 2000)
	Dry deposition: gases	resistance approach (Simpson et al., 2003; Emberson et al., 2000),
	Dry deposition: aerosols	gravitational settling (Simpson et al., 2003; Emberson et al., 2000),
	Wet deposition	Simpson et al. (2003)
<b>Assimilation</b>	Assimilation method	Intermittent 3D-Var
	Assimilated surface pollutants	NO <sub>2</sub> , O <sub>3</sub> , CO, SO <sub>2</sub> , PM <sub>2.5</sub> , PM <sub>10</sub>
	assimilated satellite	none
	Frequency of assimilation	Hourly

## 1.2 Model Overview

The Danish Eulerian Hemispheric Model (DEHM) is a 3-dimensional, offline, large-scale, Eulerian, atmospheric chemistry transport model developed to study long-range transport of

air pollution in the Northern Hemisphere. DEHM was originally developed in the early 1990's in order to study the atmospheric transport of sulphur-dioxide and sulphate into the Arctic (Christensen, 1997; Heidam et al., 2004). The model has been modified, extended and updated continuously since then and now includes a flexible setup with the possibility for nested domains with higher resolutions over targeted areas (e.g. Brandt et al., 2012, Geels et al., 2021). Apart from standard air pollution components and pollen the DEHM model also includes mercury CO<sub>2</sub> (Lansø et al., 2019) and POPs (Hansen et al., 2008).

### **1.3 Model geometry**

The horizontal domain is defined on a regular latitude-longitude grid of 0.1° resolution covering longitude 24.95°W to 44.95°E and latitude 30.05°N to 71.95°N. The vertical discretization is defined on 29 terrain-following sigma levels up to about 100hPa. The 12 lowest layers are within the lowest 1 km of the atmosphere and the thickness of the lowest layer is about 20m. The model includes an option for downscaling to the surface, but this is not applied in the operational setup.

### **1.4 Forcing Meteorology**

The forcing meteorology is retrieved from the IFS model vertical layers covering the DEHM vertical extent on a 0.2°x0.2° horizontal grid resolution with a temporal resolution of 3 hours. The forecast released at 12:00UTC of the previous days is used. The meteorological parameters included to force the DEHM forecast are: 3D fields of the horizontal wind components (U,V), temperature, specific humidity, cloud liquid water contents, cloud ice water contents, rain water contents, snow water contents and fraction of cloud cover. The 2D fields are land-sea mask, surface pressure, geopotential height, skin temperature, Ustar, large scale and convective rain, snow depth, sensible heat flux, latent heat flux, net solar radiation, boundary layer height, 2m temperature, 2m dew point temperature, 10 m wind (U,V), albedo, sea ice area fraction and surface roughness.

### **1.5 Chemical initial and boundary conditions**

Lateral and top boundary conditions are taken from chemical species available in the global IFS forecast model of the previous day at 3hr temporal resolution. The DEHM forecasts are initialised by the DEHM forecasts of the previous day.

### **1.6 Emissions**

The common annual anthropogenic emissions CAMS-REG are implemented as explained in Section 3.2. Originally the temporal disaggregation was based on the GENEMIS tables, using a GNFR to SNAP matrix. From 2021 the new CAMS-TEMPO (Guevara et al., 2021) profiles for annual, monthly, weekly and daily distribution of emissions have been included in the operational version of DEHM. PM components are speciated using the splits provided with the CAMS-REG emissions. The speciation of VOCs from the emission input of total non-methane VOCs is based on the global speciated NMVOC emission database EDGAR 4.3.2 (Huang et al., 2017).

Natural emissions of the Biogenic Volatile Organic Compounds (BVOCs) isoprene and monoterpenes are estimated in the DEHM model based on the MEGAN model (Zara et al. 2012). The production of sea salt aerosols at the ocean surface is based on two

parameterisation schemes describing the bubble-mediated sea spray production of smaller and larger aerosols. In each time step, the production is calculated for 10 size bins and thereafter summed up to give an aggregated production of fine (with dry diameters <1.3  $\mu\text{m}$ ) and coarse (with dry diameters ranging 1.3-6 $\mu\text{m}$ ) aerosols (Soares et al. 2016). Soil and lightning NO<sub>x</sub> emissions are based on data from the Global Emissions Inventory Activity (GEIA; (Yienger and Levy, 1995).

The hourly GFAS wildfire emissions are retrieved as soon as they are available (i.e. with a 8-hr delay from real time) in order to obtain a recent 24hr cycle spanning over D-2 and D-1. This cycle is used for the analysis (D-1) and the first two days of the forecast (D+0 and D+1). Fire emissions are set to zero for the remainder of the forecast horizon. Hourly injection heights are calculated based on the hourly data of 'Mean altitude of maximum injection' and 'Altitude of plume top'.

### **1.7 Solver, advection and mixing**

The horizontal advection is solved numerically using the higher order Accurate Space Derivatives scheme, documented to be very accurate (Dabdub and Seinfeld, 1994), especially when implemented in combination with a Forester filter (Forester, 1977). The vertical advection as well as the dispersion sub-models is solved using a finite elements scheme (Pepper et al., 1979) for the spatial discretization. For the temporal integration of the dispersion, the q-method (Lambert, 1991) is applied and the temporal integration of the 3 dimensional advection is carried out using a Taylor series expansion to third order. Time integration of the advection is controlled by the Courant-Friedrich-Lewy (CFL) stability criterion. A wind adjustment is included in order to ensure mass conservation.

The vertical diffusion is configured by K<sub>z</sub> profiles (Hertel et al., 1995), based on Monin-Obukhov similarity theory for the surface layer. This K<sub>z</sub> profile is extended to the whole boundary layer by using a simple extrapolation, which ensures that K<sub>z</sub> is decreasing in the upper part of the boundary layer. The planetary boundary layer (PBL) height is obtained directly from the IFS meteorology.

### **1.8 Deposition**

Gaseous and aerosol dry-deposition velocities are calculated based on the resistance method for 16 different land-use types and are configured similar to the EMEP model (Simpson et al., 2003; Emberson et al., 2000), except for the dry deposition of species on water surfaces, where the deposition depends on the solubility of the chemical species and the wind speed (Hertel et al., 1995).

Wet deposition includes in-cloud and below-cloud scavenging and is calculated as the product of scavenging coefficients and the concentration of gases and particles in air (Simpson et al. 2003). The in-cloud scavenging coefficients are dependent on Henry's law constants and the rate at which precipitation is formed.

### **1.9 Chemistry and aerosols**

The basic chemical scheme in DEHM now includes 74 different species and 158 reactions. It is based on the original scheme by Strand and Hov (1994). The original Strand and Hov scheme has been modified in order to improve the description of, amongst other things, the transformations of nitrogen containing compounds. The chemical scheme has been extended

with a detailed description of the ammonia chemistry through the inclusion of ammonia ( $\text{NH}_3$ ) and related species: ammonium-nitrate ( $\text{NH}_4\text{NO}_3$ ), ammonium bisulphate ( $\text{NH}_4\text{HSO}_4$ ), ammonium sulphate ( $(\text{NH}_4)_2\text{SO}_4$ ) and particulate nitrate ( $\text{NO}_3$ ) formed from nitric acid ( $\text{HNO}_3$ ) using an aerosol equilibrium approach with reaction rates dependent on the equilibrium (Frohn, 2004). Furthermore, reactions concerning the wet-phase production of particulate sulphate have been included. The photolysis rates are calculated by using a 2-stream version of the Phodis model (Kylling et al., 1995). The original rates for inorganic and organic chemistry have been updated with rates from the chemical scheme applied in the EMEP model (Simpson et al., 2003). SOA formation is included via a VBS-based approach (Zare et al. 2014; Bergström et al., 2012). In total, DEHM includes nine classes of particulate matter (PM<sub>2.5</sub>, PM<sub>10</sub>, TSP, seasalt < 2.5 mm, sea-salt > 2.5 mm, smoke from wood stoves, fresh black carbon, aged black carbon, and organic carbon).

### **1.10 Assimilation system**

Since the system upgrade in November 2020, the assimilation in DEHM has been based on an updated version of the comprehensive 3D-var data assimilation scheme previously described in Silver et al. (2016). The NMC method (Parish and Derber, 1992; Kahnert, 2008) is used to estimate the background error covariance matrix. Two 1-year runs of DEHM using analysed and forecasted ECMWF weather data are performed and their differences are used to estimate the background errors in spectral space for O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, CO, PM<sub>2.5</sub>, and PM<sub>10</sub>. For the analysis and reanalysis runs, surface in-situ observations of the six species are assimilated at an hourly basis in DEHM. In order to optimise runtime, and also considering the good performances achieved, only daytime observations (8:00-19:00 UTC) are assimilated for O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, CO, and all-day observations are assimilated for PM<sub>2.5</sub>, and PM<sub>10</sub>.